

Tetraethylenepentamine  
112-57-2 | DTXSID7026108

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.47 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.70 \times 10^{-1}$

**Confidence level:**  $7.79 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

Hexadecane

**Measured:**  $2.49 \times 10^{-11}$

**Predicted:**  $2.20 \times 10^{-11}$

Image not found

Pentadecane

**Measured:**  $2.22 \times 10^{-11}$

**Predicted:**  $2.07 \times 10^{-11}$

Image not found

2-(2-Butoxyethoxy)ethanol

**Measured:**  $7.44 \times 10^{-11}$

**Predicted:**  $5.15 \times 10^{-11}$

Image not found

Tetradecane

**Measured:**  $1.92 \times 10^{-11}$

**Predicted:**  $1.90 \times 10^{-11}$

Image not found

Simazine

**Measured:**  $1.10 \times 10^{-11}$

**Predicted:**  $1.22 \times 10^{-11}$